X-Ray Diffraction of Table Salt and Potassium Chloride

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Presentation Overview

1. X-Ray Diffraction Theory
   - What is X-Ray Diffraction? How is it used?
2. Experimental Set-Up
   - How was the experiment set up?
3. Data and Discussion
   - How the data was used and what results we got.
4. Conclusion

Purpose

The purpose of this experiment is to find the lattice constant of table salt and potassium chloride.

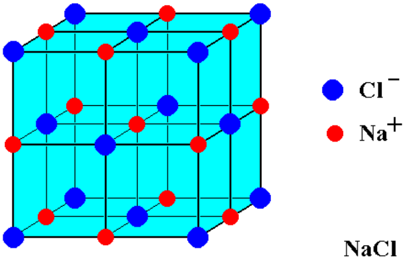

Figure: Simple face centered cubic structure unit cell. Particularly this is a piece of table of table at the smallest scale.

X-Ray Diffraction Theory

Generic X-Ray Diffraction can be seen in the following Figure [4].

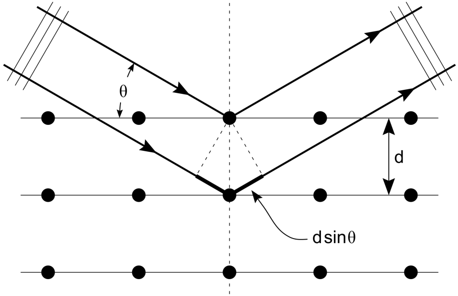

Figure: X-Ray Diffraction of a lattice structure.

The θ angle can be measured with the use of a diffractometer.

Equipment Used

- Rigaku Miniflex X-Ray Diffractometer

- Glass Slide
- Ethyl Alcohol
- Table salt and Potassium Chloride

Experimental Set-Up

First the Rigaku Miniflex had to be turned on with the cooling system. A small sample of table salt or potassium chloride was put on the glass with ethyl alcohol used to keep the sample on the glass slide.

After the slide was placed inside the Rigaku Miniflex, the diffractometer started sending X-Rays that were to be incident on the sample placed inside.

Data and Discussion

By knowing the angle of diffraction, Bragg's law can be used to identify the lattice spacing between atoms and eventually the lattice constant. The equation for Bragg's law is [1]

$$2d \sin \theta = n\lambda. \tag{1}$$

The equation for how the lattice constant is calculated with the atom spacing d is [2]

$$a = d\sqrt{h^2 + k^2 + l^2}. \tag{2}$$

The h,k,l that show up in equation (2) are known as Miller indices. These value are specific for a certain geometry.

To get a better understanding of what Miller indices are, the following figure can depict this [3].

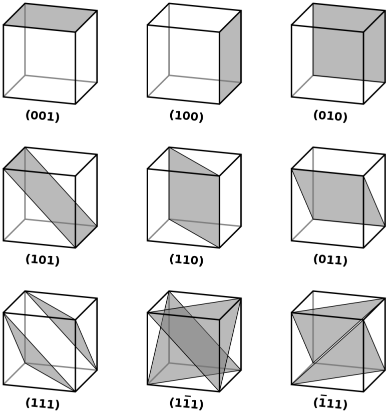

Figure: Visual representation of Miller indices.

Data and Discussion

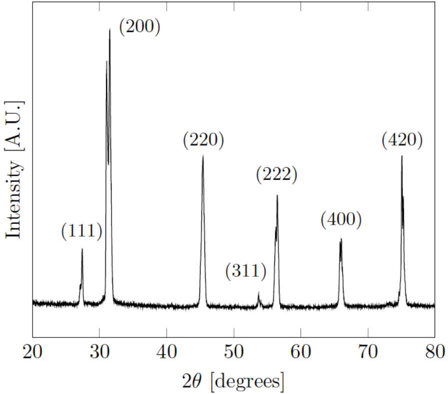

Figure: X-Ray diffraction pattern for table salt. The diffraction patterns are graphed against 2θ because of the instrumentation set up. It was essential that 2θ was measured not just θ. The Miller Indices found in the pattern come from peer reviewed papers where some come from hand calculations.

The table below depicts the data that was found in the diffraction pattern for table salt.

Peak	Diffraction Angle 2θ ^{o}	Intensity	Distance Between Planes "d" nm	Lattice Constant "a" nm
(111)	27.35	126.7±4.850	0.326	0.565
(200)	31.39	303.7±13.74	0.285	0.570
(220)	45.39	654.9±9.580	0.200	0.566
(311)	53.80	37.2±3.26	0.171	0.567
(222)	56.39	471.4±8.170	0.163	0.566
(400)	65.98	284.1±6.610	0.142	0.567
(420)	75.15	475.9±8.390	0.127	0.566

Table: XRD data for table salt.

Data and Discussion

With the data found in the previous table we can report a final value for the lattice constant of table salt. Our final value for the lattice constant of table salt is

$$a_{NaCl} = 0.567(1)\ nm. \tag{3}$$

The formal value for the lattice constant of table salt is [2]

$$a_{NaCl} = 0.564\ nm. \tag{4}$$

Immediate observations show that our calculated value is not in the range of the formal value. We now wish to report the lattice constant for potassium chloride.

Data and Discussion

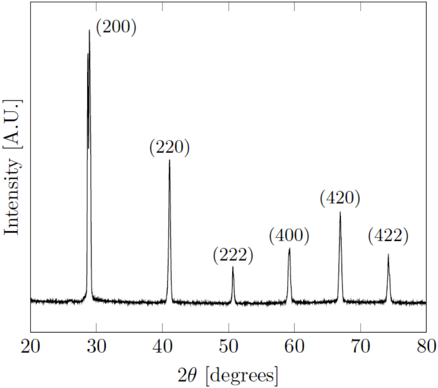

Figure: X-Ray diffraction of potassium chloride. Most of the Miller Indices were cross referenced with peer reviewed data to ensure accuracy. We once again had to calculate some of the Miller Indices by hand.

Data and Discussion

The data for the potassium chloride X-Ray diffraction can be seen in the table below.

Peak	Diffraction Angle 2θ ^{o}	Intensity	Distance Between Planes "d" nm	Lattice Constant "a" nm
(200)	28.89	1847.8$\pm$50.546	0.309	0.618
(220)	41.07	730.8$\pm$32.23	0.220	0.622
(222)	50.70	151.2$\pm$15.98	0.180	0.624
(400)	59.21	356.6$\pm$23.45	0.156	0.624
(420)	66.94	572.8$\pm$28.93	0.140	0.626
(422)	74.25	275.1$\pm$20.96	0.128	0.627

Table: XRD data for potassium chloride..

Data and Discussion

Paralleled to table salt, the lattice constant for potassium chloride from our experiment was finally

$$a_{KCl} = 0.624(3)\ nm. \tag{5}$$

The formal value for the lattice constant of potassium chloride is [2]

$$a_{KCl} = 0.629\ nm. \tag{6}$$

We once again can see that our calculated value for the lattice constant is slightly off from the formal value.

Conclusion

- Calculated values are slightly off from those that were referenced.
- The main contributor to the errors in this lab were systematic. i.e the equipment we were using needed to be calibrated.
- Not every piece of salt is going to be the same size, the lattice constant should be interpreted as an average for one length of the unit cell, not an official one.

References

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